

Search Overview

Search: search1
Date/Time done: Fri Jul 08 15:38:54 2016
Database(s): CSD version 5.37 updates (Nov 2015)
CSD version 5.37 (November 2015)
CSD version 5.37 (November 2015)
CSD version 5.37 updates (Feb 2016)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 8

Single query used. Search found structures that:

match

Query 1

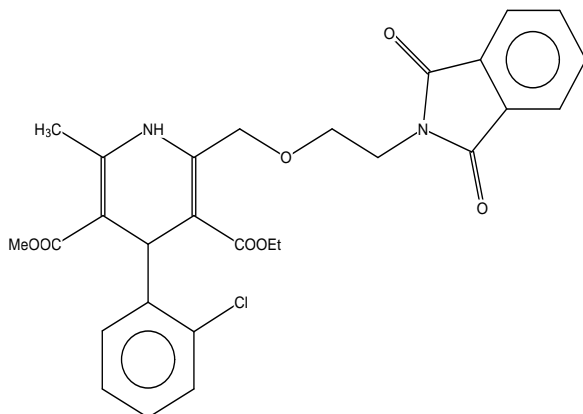
Query 1

Name **amlodipine**

Search: search1 (Fri Jul 08 15:38:54 2016): Hits 1-4

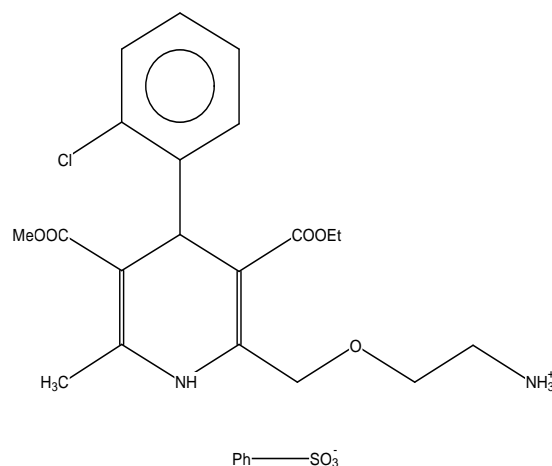
FAYGES

Reference:	H.S.Yathirajan, B.Nagaraj, M.Bolte (2005) <i>Acta Crystallogr., Sect.E: Struct. Rep. Online</i> , 61 ,o174					
Formula:	C ₂₈ H ₂₇ Cl ₁ N ₂ O ₇					
Compound Name:	Ethyl methyl (4 <i>RS</i>)-4-(2-chlorophenyl)-2-(((2-(1,3-dioxo-1,3-dihydro-2 <i>H</i> -isoindol-2-yl)ethyl)oxy)methyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate					
Synonym:	Phthaloyl amlodipine					
Space Group:	P-1	Cell:	a	b	c	
Space Group No.:	2	(Å, °)	8.046(0)	10.519(1)	15.739(1)	
			α 98.07(0)	β 90.54(0)	γ 103.74(0)	
R-Factor (%) :	3.37	Temperature(K) :	173	Density(g/cm³) :	1.399	



INEDUB

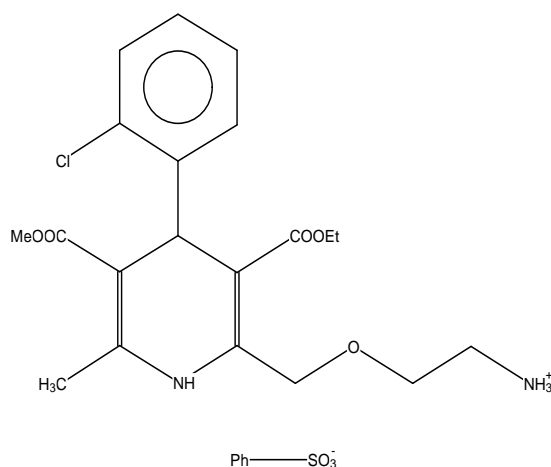
Reference:	V.Koradia, H.L.de Diego, K.Frydenvang, M.Ringkjobing-Elema, A.Mullertz, A.D.Bond, J.Rantanen (2010) <i>Cryst.Growth Des.</i> , 10 ,5279					
Formula:	C ₂₀ H ₂₆ Cl ₁ N ₂ O ₅ S ₁ 1 ⁺ ·2(H ₂ O ₁)					
Compound Name:	Amlodipine besylate dihydrate					
Synonym:	2-((4-(2-Chlorophenyl)-3-(ethoxycarbonyl)-5-(methoxycarbonyl)-6-methyl-1,4-dihydropyridin-2-yl)methoxy)ethanaminium benzenesulfonate dihydrate					
Space Group:	P21/c	Cell:	a	b	c	
Space Group No.:	14	(Å, °)	18.892(2)	9.507(0)	16.357(3)	
			α 90.00	β 105.28(1)	γ 90.00	
R-Factor (%) :	3.27	Temperature(K) :	122	Density(g/cm³) :	1.414	



H₂O

INEDUB01

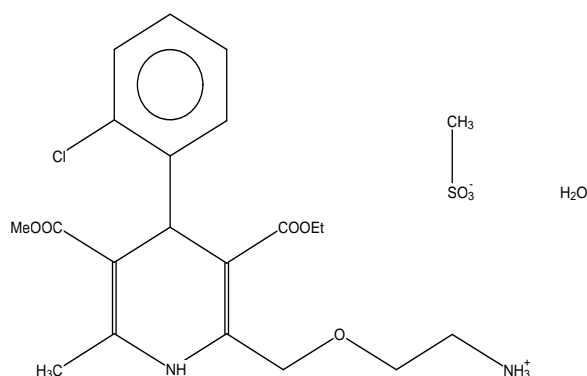
Reference:	V.Koradia, H.L.de Diego, K.Frydenvang, M.Ringkjobing-Elema, A.Mullertz, A.D.Bond, J.Rantanen (2010) <i>Cryst.Growth Des.</i> , 10 ,5279					
Formula:	C ₂₀ H ₂₆ Cl ₁ N ₂ O ₅ S ₁ 1 ⁺ ·2(H ₂ O ₁)					
Compound Name:	Amlodipine besylate dihydrate					
Synonym:	2-((4-(2-Chlorophenyl)-3-(ethoxycarbonyl)-5-(methoxycarbonyl)-6-methyl-1,4-dihydropyridin-2-yl)methoxy)ethanaminium benzenesulfonate dihydrate					
Space Group:	P21/c	Cell:	a	b	c	
Space Group No.:	14	(Å, °)	19.110(1)	9.624(0)	16.693(1)	
			α 90.00	β 106.69(0)	γ 90.00	
R-Factor (%) :	4.25	Temperature(K) :	293	Density(g/cm³) :	1.362	



H₂O

NERXIS

Reference:	R.J.Butcher, R.S.Narasegowda, H.S.Yathirajan, H.G.Anilkumar, B.Narayana (2006) <i>Acta Crystallogr., Sect.E: Struct. Rep. Online</i> , 62 ,o5814					
Formula:	C ₂₀ H ₂₆ Cl ₁ N ₂ O ₅ S ₁ 1 ⁺ ·C ₁ H ₃ O ₃ S ₁ 1 ⁻ ·H ₂ O ₁					
Compound Name:	(R,S)-3-Ethyl 5-methyl 2-(2-ammonioethoxymethyl)-4-(2-chlorophenyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate methanesulfonate monohydrate					
Synonym:	Amlodipine mesylate monohydrate					
Space Group:	C2/c	Cell:	a	b	c	
Space Group No.:	15	(Å, °)	47.656(11)	11.069(2)	9.848(2)	
			α 90.00	β 99.56(0)	γ 90.00	
R-Factor (%) :	4.76	Temperature(K) :	298	Density(g/cm³) :	1.356	



Search: search1 (Fri Jul 08 15:38:54 2016): Hits 5-8

PALNOF

Reference: S.Goldmann, J.Stoltefuss, L.Born (1992) *J.Med.Chem.* ,**35**, 3341

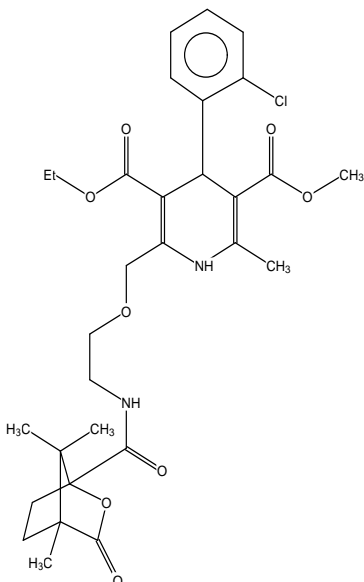
Formula: C₃₀ H₃₇ Cl₁ N₂ O₈

Compound Name: 4S-2-(((2-Camphanoylamino)ethoxy)methyl)-4-(2-chlorophenyl)-3-ethoxycarbonyl-5-methoxycarbonyl-6-methyl-1,4-dihydropyridine

Synonym: (1S)-Camphanoyl-(-)-4S-amlopidine

Space Group: P21 **Cell:** *a* 11.744(3) *b* 9.013(2) *c* 14.347(3)
Space Group No.: 4 **Cell:** (Å, °) *α* 90.00 *β* 99.48(3) *γ* 90.00

R-Factor (%): 8.70 **Temperature(K)**: 295 **Density(g/cm³)**: 1.306



PALNUL

Reference: S.Goldmann, J.Stoltefuss, L.Born (1992) *J.Med.Chem.* ,**35**, 3341

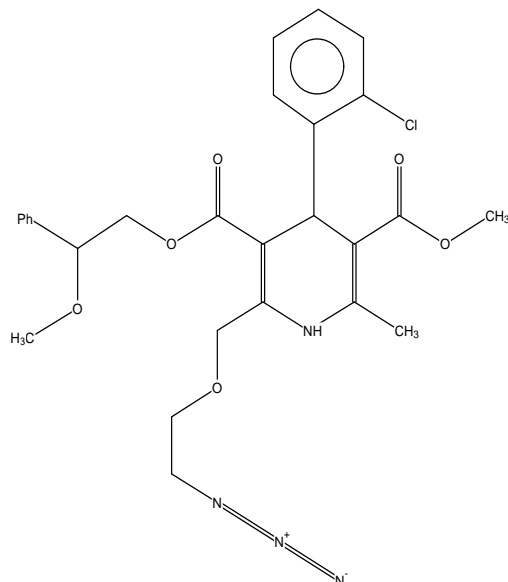
Formula: C₂₇ H₂₉ Cl₁ N₄ O₆

Compound Name: 2-((2-Azidoethoxy)methyl)-4-(2-chlorophenyl)-5-(methoxycarbonyl)-3-((2S)-methoxy-2-phenethoxy)carbonyl)-6-methyl-1,4-dihydropyridine

Synonym: 3-((S)-2-Methoxy-2-phenethoxy)carbonyl)-(-)-4S-amlopidine

Space Group: P212121 **Cell:** *a* 7.699(2) *b* 11.842(6) *c* 29.224(4)
Space Group No.: 19 **Cell:** (Å, °) *α* 90.00 *β* 90.00 *γ* 90.00

R-Factor (%): 5.70 **Temperature(K)**: 295 **Density(g/cm³)**: 1.349



VAWPOZ

Reference: R.Banjeree, P.M.Bhatt, N.V.Ravindra, G.R.Desiraju (2005) *Cryst.Growth Des.* ,**5**,2299

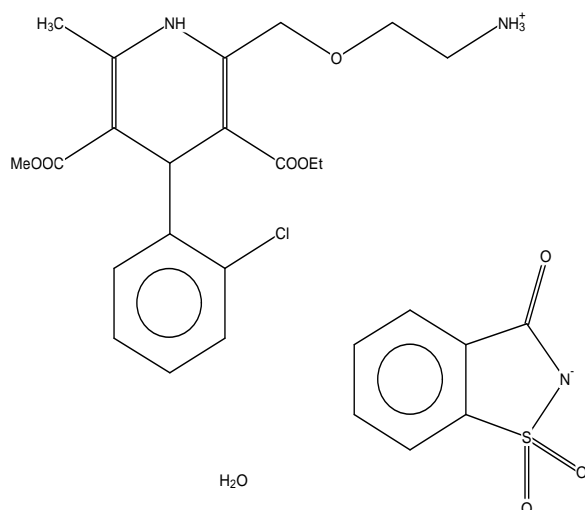
Formula: C₂₀ H₂₆ Cl₁ N₂ O₅ 1⁺.C₇ H₄ N₁ O₃ S₁ 1⁻.H₂ O₁

Compound Name: 3-Ethyl 5-methyl 2-((2-ammonioethoxy)methyl)-4-(2-chlorophenyl)-1,4-dihydro-6-methyl-3,5-pyridinedicarboxylate 2,3-dihydro-3-oxobenzisulfonazolate monohydrate

Synonym: Amlodipine saccharinate monohydrate

Space Group: P-1 **Cell:** *a* 7.807(0) *b* 7.933(0) *c* 24.745(2)
Space Group No.: 2 **Cell:** (Å, °) *α* 97.19(0) *β* 93.03(0) *γ* 112.63(0)

R-Factor (%): 13.42 **Temperature(K)**: 100 **Density(g/cm³)**: 1.453



XOZRUI

Reference: K.Mereiter, J.Rollinger (2002) *CSD Communication(Private Communication)* ,

Formula: C₂₀ H₂₆ Cl₁ N₂ O₅ 1⁺.C₆ H₅ O₃ S₁ 1⁻

Compound Name: Amlodipine besylate

Synonym: 2-((2-Ammonioethoxy)methyl)-4-(2-chlorophenyl)-5-(methoxycarbonyl)-3-(ethoxycarbonyl)-6-methyl-1,4-dihydropyridine benzenesulfonate

Space Group: Pbca **Cell:** *a* 10.121(4) *b* 18.341(6) *c* 30.518(10)
Space Group No.: 61 **Cell:** (Å, °) *α* 90.00 *β* 90.00 *γ* 90.00

R-Factor (%): 5.97 **Temperature(K)**: 297 **Density(g/cm³)**: 1.330

